

1-Butanol
71-36-3 | DTXSID1021740

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.35 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.10e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

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1-Butanol

Measured: 8.53e-01

Predicted: 1.35

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2-Methyl-1-propanol

Measured: 1.15

Predicted: 1.50

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Pent-4-en-1-ol

Measured: 6.62e-01

Predicted: 5.01e-01

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But-2-en-1-ol

Measured: 13.9

Predicted: 6.02

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2-Butanol

Measured: 2.44

Predicted: 1.98